ABSTRACT OF THE DISCLOSURE

Provided herein are computer-based methods for generating and using three-dimensional (3-D) structural models of target biomolecules. In particular, the target biomolecules are protein structural variants derived yfrom genes containing genetic variations, or polymorphisms. The models are generated using molecular modeling techniques, such as homology modeling. The models can be used in structure-based drug design studies to identify drugs that bind to particular structural variants in structure-based drug design studies, for designing allele-specific drugs, population-specific drugs and for predicting clinical responses in patients. Molecular structure databases containing protein structural variant models are also provided.